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Spatially resolved mass transfer coefficient for moderate Reynolds number flows in packed beds: Wall effects

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ABSTRACT

In this paper, Direct Numerical Simulation (DNS) was performed to understand the effects of confining walls on mass transfer through a packed bed for laminar regime ($Re \leq 100$). The *X*, *Y* and *Z* coordinates of the center of the spheres in a randomly packed bed with varying ratios D/d (*D* is the diameter of the column and *d* is the diameter of the particle) were generated using a Discrete Element Method - Computational Fluid Dynamics (DEM-CFD) code. Naphthalene-air system ($Sc \sim 2.52$) was considered for all the cases. The grid resolution, method and boundary conditions were validated by comparing the computed (overall) Sherwood number with the published experimental data. Local Sherwood number was computed around each particle for all ratios, D/d, and spatial and probability distributions throughout the packed bed column as a function of D/d are reported. It was observed that for D/d's ≤ 8.6, the effects of wall on particle's Sherwood number was evident, while for D/d's ≥ 10.8, the Sherwood number was predominantly uniform all through the column.

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1. Introduction

Packed bed contactors have been extensively utilized as a part of industrial applications for several decades. They are used to enhance contact between two phases in many chemical separation processes such as absorption, stripping and distillation. Despite new contactor designs have been introduced, packed bed contactors are still widely utilized [1], principally owing to their simple design and low cost.

An important transport phenomenon to consider while designing and operating a packed bed contactor is mass transfer. Hence, accurate estimation of mass transfer coefficient is essential. Several empirical correlations have been published in the literature to determine the mass transfer coefficient for both a single particle and/or arrays of particles as observed in packed bed contactors [2,3]. These correlations are useful, from an engineer's perspective, as they give quick estimates of average mass transfer rates to design a packed bed. However, they don't provide the information on the spatial distribution of mass transfer rates in such a bed.

To accurately estimate the mass transfer rate in a packed bed contactor, the fluid-particle interactions should be fully resolved both spatially and temporally. Unlike continuum models such as Euler-Euler model that is used by practicing engineers, Direct Numerical Simulation (DNS) is a useful tool that can be used to precisely determine the fluid-particle interactions and develop a closure for many continuum models' terms. The computational cost of DNS is very high and therefore, it is typically possible to perform DNS for systems of $O(10^3)$ particles simultaneously. However, this barrier has been alleviated by a steady increase in computational power.

Most DNS studies of dense fluid-particle systems have been restricted to momentum transfer. For instance, Beetstra et al. [4,5], Hoef et al. [6], and Hill et al. [7] presented drag relations derived from lattice-Boltzmann (LBM) simulations. Feng and Michaelides [8] reported an effective velocity updating scheme for LBM-simulations of particulate flows. Recently, DNS studies of dense fluid-particle systems have been extended to include heat transfer. Dan and Wachs [9], Deen et al. [10], Nijemeisland and Dixon [11], Shao et al. [12], and Wachs [13] performed DNS of heat transfer in particulate flows. Feng and Michaelides [14], Yang et al. [15], and Yang et al. [16] studied dynamics of non-isothermal non-spherical particulate flows through DNS. Some studies have

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Nomenclature

D	column diameter (m)
d	particle diameter (m)
v	superficial velocity (m/s)
p	pressure (N/m^2)
F	volumetric flow rate (m^3/s)
S	surface area (m^2)
S_{total}	total surface area of the active packing material (m^2)
V	volume (m^3)
R_p	particle radius (m)
$D_{A,f}$	diffusivity of species A (m^2/s)
$C_{A,f}$	concentration of species A (kg/m^3)
$c_{A,f}$	bulk concentration of species A (kg/m^3)
$C_{A,in}$	inlet concentration of species A (kg/m^3)
$C_{A,out}$	outlet concentration of species A (kg/m^3)
$C_{A,s}$	surface concentration of species A (kg/m^3)
k_o	overall mass transfer coefficient (m/s)
k_L	overall mass transfer coefficient (m/s)
$Re = \frac{\rho_f v d}{\mu_f}$	Reynolds number (dimensionless)
$Sc = \frac{\mu_f}{\rho_f D_{A,f}}$	Schmidt number (dimensionless)
Sh_o	overall Sherwood number (dimensionless)
Sh_L	local Sherwood number (dimensionless)

Greek letters

μ_f	dynamic viscosity (kg/m s)
ρ_f	density (kg/m^3)
β	scaling factor
Ψ	area averaged mass flux (kg/m^2 s)
Φ	concentration difference (kg/m^3)

Vectors

$\bar{g}$	gravitational acceleration (m/s^2)
$\bar{u}$	velocity (m/s)
$\bar{r}$	position vector (m)

Subscripts and Superscripts

f	fluid phase
p	particle

Operators

$\frac{\partial}{\partial t}$	partial time derivative (1/s)
$\frac{\partial}{\partial r}$	partial radial derivative (1/m)
∇	gradient operator (1/m)
∇	divergence operator (1/m)
∇^2	Laplace operator (1/m^2)

focused on combined effect of momentum, mass and heat transfer. For example, Dierich et al. [17] performed DNS in 2D to understand the dynamics of particulate flows undergoing phase change along with interfacial heat transfer on the particle surface. Dierich and Nikrityuk [18] used Euler-Lagrange method in 2D to capture phase change effect in particulate flows. Li et al. [19] investigated the complex process of endothermal catalytic reaction in catalyst porous media using LBM-method. Recently, Deen and Kuipers [20] used novel Immerse Boundary Method (IBM) to couple heat and mass transfer in dense fluid particle systems.

Both experimental and numerical investigations have been carried out to understand the mass transfer phenomenon in dense fluid particle systems. Dwivedi and Upadhyay [2], and Wakao and Funazkri [3] published comprehensive reviews on mass transfer in packed beds. Tsotsas and Schlünder [21] studied experimentally mass transfer through a packed bed for very low ratios of tube to particle diameter (D/d). Atmakidis and Kenig [22] performed numerical analysis of mass transfer in packed beds with irregular particle arrangements. Empirical correlations published in the literature are generally developed for large D/d ratios, where wall effects are negligible. Packed bed reactors with smaller values of D/d (<5) are usually used for highly exothermic heterogeneous catalytic reactions, where wall effects are significant. The application of empirical correlations, published for large values of D/d ratios, to design a packed bed with small values of D/d ratios would lead to substantial inaccuracies. Hence, wall effects play an important role in hydrodynamics and mass transfer through a packed bed. In order to study wall effects along with an accurate determination of the spatial distributions of mass transfer rates through packed beds, DNS must be performed. Deen and Kuipers [23] performed DNS to predict the spatial distribution of mass transfer coefficient in dense gas-particle arrays at low to moderate Reynolds number (Re), but the influence of confining walls was not investigated.

The objective of this study is to perform DNS to study the effect of confining walls on mass transfer in a packed bed for laminar regime ($Re \leq 100$) and accurately predict the 'local' mass transfer coefficient around each particle in such a bed at such a flow regime. Packed beds are of high industrial importance and are mostly cylindrical in nature hence the choice of a cylindrical column. The probability distribution curve and spatial distribution of mass transfer rates in a packed bed are evaluated. Our aim is to perform packed bed simulations for as realistic geometry as possible. In reality, packed beds are generally randomly packed. Hence, randomly packed bed configuration will be studied, and no unit cell configurations (FCC, BCC, HCP, etc.) will be considered. Previous studies on mass transfer through randomly packed bed created the geometry of their systems using Monte Carlo method while our geometry was developed using DEM-CFD method. The latter ensures a more realistic geometry of a randomly packed bed.

The structure of the paper is as follow. First, the description of the geometry studied is presented. Next, the model description and implementation are detailed. Finally, the results and discussion consisting of grid and method validation, and wall effects are discussed.

2. Geometry description

In Fig. 1, the representative snapshots of the packed bed column geometry with D/d equal to 6.4, 8.6, and 16.5 are presented. The X, Y and Z coordinate of the center of spherical particles in a packed bed is generated using a Discrete Element Method - Computational Fluid Dynamics (DEM-CFD) code [24]. The code is a two-way coupled particle dynamics solver that uses the volume-averaged Navier-Stokes equation to solve the fluid field equations in addition to the DEM that tracks translational and rotational particle motion. At the beginning of the simulation, the particles are initialized in a regular lattice with a given density and size. The domain, referred hereafter as "randomization domain" and in which the particles are initialized, is of the same size as the cylindrical domain used in the DNS but the length is made 4 times longer than the DNS domain in order to allow the displacement of particles due to fluidization. The inlet at the bottom of the randomization domain is maintained as a velocity inlet, while the pressure boundary condition is set for the top of the domain. Based on particles density and size, the minimum fluidization velocity is computed from fluidization theory [25]. Twice the minimum fluidization

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